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Title: GASFLOW: A COMPUTATIONAL MODEL TO ANALYZE ACCIDENTS IN NUCLEAR CONTAINMENT AND FACILITY BUILDINGS

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GASFLOW: A Computational Model to Analyze Accidents in Nuclear Containment and Facility Buildings

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ABSTRACT

GASFLOW is a finite-volume computer code that solves the time-dependent, compressible Navier-Stokes equations for multiple gas species. The fluid-dynamics algorithm is coupled to the chemical kinetics of combusting liquids or gases to simulate diffusion or propagating flames in complex geometries of nuclear containment or confinement and facilities' buildings. Fluid turbulence is calculated to enhance the transport and mixing of gases in rooms and volumes that may be connected by a ventilation system. The ventilation system may consist of extensive ductwork, filters, dampers or valves, and fans. Condensation and heat transfer to walls, floors, ceilings, and internal structures are calculated to model the appropriate energy sinks. Solid and liquid aerosol behavior is simulated to give the time and space inventory of radionuclides. The solution procedure of the governing equations is a modified Los Alamos ICE'd-ALE methodology.

Complex facilities can be represented by separate computational domains (multiblocks) that communicate through overlapping boundary conditions. The ventilation system is superimposed throughout the multiblock mesh. Gas mixtures and aerosols are transported through the free three-dimensional volumes and the restricted one-dimensional ventilation components as the accident and fluid flow fields evolve. Combustion may occur if sufficient fuel and reactant or oxidizer are present and have an ignition source. Pressure and thermal loads on the building, structural components, and safety-related equipment can be determined for specific accident scenarios.

GASFLOW calculations have been compared with large oil-pool fire tests in the 1986 HDR containment test T52.14, which is a 3000-kW fire experiment. The computed results are in good agreement with the observed data.

I. INTRODUCTION

The occurrence of a number of severe fire accidents in nuclear facilities has motivated research activities to model combustion phenomena in these systems. The most publicized accidents are the electrical wire insulation (cable tray) fire at the Brown's Ferry nuclear power plant[1] and the hydrogen combustion event during the Three Mile Island accident.[2] Severe fires involving small radiation confinement compartments (glove boxes) and high efficiency particulate air (HEPA) filters have occurred in the Rocky Flats facility.[3] Significant, but less severe, flammable liquid fires have occurred in diesel generator rooms and turbines.[4]

It is important to analyze entire facilities to determine the transient pressure and heating loads due to combustion events on the containment or ventilation structures and safety related equipment. These analyses are also needed to plan emergency evacuation, to validate existing fire protection programs or suggested changes, and to integrate fire safety with other safety analysis requirements. The US Nuclear Regulatory Commission and the US Department of Energy are supporting research at Los Alamos to develop a state of the art, best estimate, transient, three dimensional computer code to evaluate threats to the nuclear reactor containments and facility buildings. We describe the Los Alamos field model approach, the GASFLOW code, in sections II and III and discuss it's application to a full scale fire experiment in section IV.

II. MATHEMATICAL AND PHYSICAL MODELS

The time-dependent, three-dimensional, compressible Navier-Stokes equations are the complete equations of motion for GASFLOW. An internal energy transport equation relates the internal energy density to the work and energy exchange functions. Multiple species transport equations model the transport of individual species through the gas mixture. The sum of the species transport equations is the total fluid density conservation equation. These equations, the Navier-Stokes equations, the internal energy equations, and the summed species transport equations, express the conservation of momentum, energy, and mass, respectively. They relate the dynamics of the fluid to temporal and spatial influences, such as, viscous stress, body force, turbulence, structural resistance, heat transfer, condensation, and combustion. Gas turbulence is simulated by either an algebraic, sub-grid scale, or k-ε turbulence model with buoyancy production terms.

The finite-volume GASFLOW code can model complex three-dimensional geometries. Structures or compartments can be represented by separate computational domains that communicate through overlapping boundary conditions. Flow between compartments is possible through one-dimensional ventilation system models. The ventilation system may be superimposed throughout the multiblock mesh. Ventilation system components include fans, dampers, and filters. Natural and forced convection may be modeled in both the one-dimensional ductwork and the three-dimensional compartments.

Heat transfer and condensation on walls and surfaces, such as, internal structures, are calculated to model appropriate energy sinks. A modified Reynolds analogy for heat and mass transport to walls and structures accounts for the influence the thermal boundary layer has on the rates of heat transfer and condensation.

Chemical kinetics models for combustion simulate diffusion and propagating flames in complex geometries. A one-step, global chemical kinetics model is often used for diffusion flames involving hydrogen or hydrocarbon fuels. This overly simplifies the actual chemical process, which has many more elementary reaction steps and intermediate chemical species. The chemical reaction time scale is, however, very short compared with fluid dynamic motions and meaningful calculations can be accomplished using this simplified chemical kinetics mechanism. The reaction rate in the finite rate chemical kinetics equations is modeled by a modified Arrhenius law that accounts for fuel lean or fuel rich mixtures.

Aerosol transport models compute the behavior of particulate matter in the gas flow fields. These one way coupled models simulate the polydisperse transport, deposition, and entrainment of discrete phase particles. The GASFLOW species transport model also functions as a continuum particle phase transport model.

III. Computational Model

The solution procedure of the governing equations is a modified Los Alamos ICE'd ALE methodology[5] for solving multidimensional, time dependent fluid flow equations. An efficient semi implicit algorithm is implemented that exploits the vector processing capability of the CRAY Y MP architecture. In the ALE method, the computational time cycle consists of three steps. Phase A is the explicit Lagrangian phase. In this phase, the density, velocity, and specific internal energy fields are updated by the effects of all chemical and physical processes. These include combustion, condensation, heat transfer, body forces, and turbulence effects. Phase B is the implicit Lagrangian phase. A solution of the momentum equations in terms of both time advanced velocities and pressures is obtained. The iteration scheme used to solve this set of equations is the preconditioned conjugate residual method that closely follows the algorithm proposed by Chandra.[6] The final phase, Phase C, is a rezone phase in which all the advective flux calculations, repartitioning of the dependent variables onto the mesh, are explicitly performed. The mesh may move with the fluid (Lagrangian), remain fixed (Eulerian), or move in any arbitrarily prescribed manner. In the GASFLOW code, the mesh remains fixed.

IV. APPLICATION TO FULL-SCALE FIRE EXPERIMENTS

We have used GASFLOW to simulate the large oil-pool fire tests in the HDR containment. For this simulation, important insight into verifying the general Navier-Stokes solution algorithm and the submodels for condensation heat transfer, turbulence, and chemical kinetics are gained.

The HDR experimental containment building is 60 m high and 20 m in diameter with a free volume of 11300 m^3 in about 70 interconnected passageways and compartments. Total interior steel surface area is in excess of 30000 m^2. The location of the oil-pool fires is between the 25-m and 30.85-m levels (measured from ground level) of the containment. Fires of 2000, 3000, and 4000 kW were burned over 30- to 35-min periods. We have calculated test T52.14, which is the 3000-kW experiment. By continuously weighing the oil pan, the rate of combustion of the hydrocarbon fuel was determined. Roughly 120 kg of fuel were consumed during the 35-min experiment.

Experimental measurements were extensive; continuous monitoring of CO_2, O_2, and H_2O concentrations, velocities, and temperatures inside, entering, and exiting, the burn compartment as well as throughout the containment itself were recorded during the entire experimental sequence. A horizontal raster or grid consisting of a 5 x 5 lattice of measuring devices was located at three separate levels above the fire level. One at the 25.5-m level is near the fresh air inlet of the mounting hatch compartment, which is connected to the combustion compartment by a door. Another at the 31-m level is at the top of the mounting hatch compartment at the entrance into the dome area. The raster at the 38-m level is inside the containment dome. In addition, video cameras were focused on key areas of the containment. More details of the experiment and the data acquisition systems is found in Ref. 7.

In general, the experimental results show that combustion occurs in the fire compartment, forming a hot layer consisting of combustion products, nitrogen, and excess oxygen (the burning occurs in an oxygen-rich environment). There is an exception to this behavior early in the experiment (3-12 min), when as a result of the feedback of combustion products into the burn room, the combustion process is fuel rich and flashover occurs with the flame spreading into the adjoining mounting hatch compartment.

Since the mass-burning rate is known, it is used as a mass and energy source for the fuel species and energy conservation equations, respectively, of the numerical model. This mass and energy fuel source is distributed uniformly in the computational cells overlaying the physical location of the oil pan. The computed gas temperature time histories from locations at the top of the combustion room and near the top of the doorway between the combustion room and the mounting hatch are in excellent agreement with the experimental values. This indicates that the overall energy released in the combustion process is modeled adequately. Comparisons between gas concentrations at the upper middle position in the burn room door indicate good agreement. The feedback and flashover trends are captured with some degree of accuracy; however, the exact production of CO_2 is off by as much as 50% during the flashover event (4-12 min) and roughly 10-15% during the more or less steady combustion process (12-35 min). Concentration measurements are a very sensitive standard for assessing the combustion model, and, in this case, the simple one-step chemical kinetics model could be modified.

The temperature measurements from the three grid locations were compared with the computed temperatures at these locations. The raster at 25.5 m corresponds to the fresh air inlet to the mounting hatch compartment. These measurements show a strong temperature distribution in this region, especially during the early part (first 10 min) of the experiment. Because of the lack of spatial resolution, the calculation is not able to resolve this distribution, but predicts more of an average during this early time. At later times, the calculation is on the high edge of the temperature distribution envelope. However, considering the spatial resolution and the complexity of the containment flow paths, we consider this comparison to be acceptable and in fair to good agreement with the experimental data.

For the raster at 31 m, where the fire plume enters the dome from the mounting hatch compartment, the early time observed and computed temperatures show that the maximum temperature of about 250 °C occurs with flashover as the flame extends high into the mounting

hatch compartment. At about 12 min, the combustion event occurs largely within the burn room. The observed temperature drops to about 160 C and gradually rises in time to 225 C just before the end of combustion. The computed temperatures drop at 12 min, but not as much as those observed. However, the computed temperatures are only slightly high from about 20 min to the end of combustion.

The raster at the 38-m level measures the temperatures in the hot-gas plume. There is a large observed temperature gradient across this plume. The calculated time histories are in excellent agreement to 9 min, reaching the maximum value at the correct time. An observed local minimum occurs at 11-12 min and the temperatures recover to near their maximum values by the end of the experiment. The computed temperatures, however, continue declining after the initial peak values. This is attributed to the fact that the algebraic turbulence model used in this calculation promotes far too much mixing and cold gases are entrained into the plume during this period, thus spreading the temperature profile beyond the observed plume width. In addition, the donor-cell advection scheme implemented for this simulation is known to be diffusive, and, therefore, numerical diffusion contributes to this effect.

V. SUMMARY

Using the GASFLOW field equation model coupled with finite-rate global chemical kinetics, we successfully analyzed hydrogen and hydrocarbon diffusion flames occurring in a nuclear reactor containment under accident conditions. These combustion modes are the easiest to model and analyze when compared with other modes of combustion, such as propagating flames in premixed fuel/oxidizer volumes.

Overall, with simplified chemical kinetics mechanisms and rather coarse spatial resolution, the calculated results are in fairly good agreement with the observed data. When fluid dynamics effects dominate the analysis with hot plumes and complex convective circulation patterns, one can often be successful calculating diffusion-type flames with simple combustion models that have been calibrated to release the correct amount of heat due to the combustion process.

References

1. Pyror, A. J., "The Brown's Ferry Nuclear Plant Fire," Society of Fire Protection Engineers, Quincy, MA, TR 77 7, 1977.

2. Henrie, J. O., and Postma, A. K., "Analysis of the Three Mile Island (TMI 2) Hydrogen Burn," *Proceedings of Second International Topical Meeting on Nuclear Reactor Thermal Hydraulics*, ANS, Hindsdale, IL, Jan. 1983, p. 1157.

3. Patterson, D. E.,"The Rocky Flats Fire," *Fire Journal*, Vol. 64, 1970, p. 5.

4. Dungan, K. N., and Lorenz, M. S., "Nuclear Power Plant Fire Loss Data," Electric Power Research Institute, Palo Alto, CA, CR EPRI NP 3179, July 1983.

5. Amsden, A. A., and Hirt, C. W., "YAQUI: An Arbitrary Lagrangian Eulerian Computer Program for Fluid Flow at All Speeds," Los Alamos Scientific Laboratory, Los Alamos, NM, Report LA 5100, March 1973.

6. Chandra, R. "Conjugate Gradient Methods for Partial Differential Equations," Ph.D. Thesis, Yale Univ., New Haven, CT, 1978.

7. Valencia, L., "Brandschutzversuche im Containment HDR Versuchsgruppe BRA Versuche TS2 1/TS2 2," Kernforschungszentrum Karlsruhe PHDR Karlsruhe, Germany, Report S 0/5/86, Feb. 1987.

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